Journal of Quality Technology
A Quarterly Journal of Methods, Applications and Related Topics

ISSN: 0022-4065 (Print) 2575-6230 (Online) Journal homepage: http://www.tandfonline.com/loi/ujqt20

A Practical Approach for Interpreting Multivariate T^2 Control Chart Signals

Robert L. Mason, Nola D. Tracy & John C. Young

To cite this article: Robert L. Mason, Nola D. Tracy & John C. Young (1997) A Practical Approach for Interpreting Multivariate T^2 Control Chart Signals, Journal of Quality Technology, 29:4, 396-406, DOI: 10.1080/00224065.1997.11979791

To link to this article: https://doi.org/10.1080/00224065.1997.11979791

Published online: 21 Feb 2018.

A Practical Approach for Interpreting Multivariate T^2 Control Chart Signals

ROBERT L. MASON

Southwest Research Institute, San Antonio, TX 78228-0510

NOLA D. TRACY and JOHN C. YOUNG

McNeese State University, Lake Charles, LA 70609-2340

A persistent problem in multivariate control chart procedures is the interpretation of a signal. Determining which variable or group of variables is contributing to the signal can be a difficult task for the practitioner. However, a procedure for decomposing the T^2 statistic into orthogonal components greatly aids the interpretation effort. In this paper, a series of examples illustrates the usefulness of this interpretation scheme and relates it to the familiar concept of a statistical distance measure. The relationship between the T^2 decomposition procedure and a regression of one variable on a subset of other variables is also demonstrated, and used to aid signal interpretation. Recommendations are made and steps are suggested to provide a faster sequential computation scheme for the decomposition.

Introduction

ONE of the major problems that arises in using a multivariate quality control chart statistic is the interpretation of a signal. This occurs primarily as a result of attempting to reduce a p-dimensional data vector into a unidimensional statistic. Such data-dimensional reduction often masks the primary causes of the signaling statistic and discourages practitioners from applying multivariate techniques.

In univariate statistical process control (SPC), a signal is produced when a new observation does not conform to the structure that is established by the historical data. Through the use of appropriate control charts, it is possible to determine if this signal is due to a shift in the process mean and/or due to a shift in the process variation. Since there is only a single variable to consider, its relationship to the other variables is ignored and thus signal interpretation is usually straightforward.

Dr. Mason is Manager of the Statistical Analysis Section. He is a Senior Member of ASQ.

Dr. Tracy is an Associate Professor of Statistics.

Dr. Young is Professor of Statistics.

In multivariate SPC, a signal can be caused by a variety of situations. For example, an observation on one of the p variables may be out of control and thus outside the bounds of process variation as established by the historical situation. Similarly, the signal may be due to a relationship between two or more of the variables which contradicts that established by the historical data. Worse yet, a signal may be produced by combinations of these two situations, with some variables being out of control and others having counter-relationships.

A common statistic used in multivariate control charts for individual observations is Hotelling's T^2, which is defined as the generalized distance from a p-dimensional sample point $\mathbf{X} = (x_1, x_2, \ldots, x_p)'$ to its sample mean. It is given by

$$T^2 = \left(\mathbf{X} - \overline{\mathbf{X}}\right)' \mathbf{S}^{-1} \left(\mathbf{X} - \overline{\mathbf{X}}\right) \tag{1}$$

where $\overline{\mathbf{X}}$ and $\mathbf{S}$ are the common estimators for the mean vector and covariance matrix obtained from a historical data set. When the observation vector, $\mathbf{X}$, is independent of the estimates $\overline{\mathbf{X}}$ and $\mathbf{S}$, the distribution of the statistic in (1) is given in (2):

$$\frac{n(n-p)}{p(n+1)(n-1)} T^2 \sim F(\alpha, p, n-p). \tag{2}$$

Many different researchers (see e.g., Jackson (1985)) have examined this statistic and demonstrated its usefulness as a charting statistic for multivariate SPC. The control chart based on it is often labeled a "multivariate Shewhart chart" to denote its similarity to a univariate Shewhart chart.

Several procedures have been developed for interpreting the T^2 statistic. The most popular involves utilizing an orthogonal decomposition of T^2 and then attempting to interpret the newly created orthogonal components. For example, we could decompose T^2 into its principal components by transforming the data from the original **X**-space to the principal component space (see e.g., Jackson (1991)). However, except in special settings (see, e.g., Tracy, Young, and Mason (1995)), it may be difficult to assign a meaningful interpretation to these principal components. More recently, Mason, Tracy and Young (1995) presented a series of orthogonal decompositions of the T^2 statistic which are easier to utilize. Their approach leads to direct interpretation of the orthogonal components involved in the decomposition. Further, it allows practitioners to assess which of the components are important or warrant detailed investigation.

The purpose of this paper is to present an improved method for interpreting the unique components resulting from applying the Mason, Tracy, and Young (1995) (hereafter MYT) decomposition to a signaling T^2 statistic. A practical approach is given with recommendations for a shortened sequential computational scheme for isolating the variables contributing to the signal.

A Bivariate Decomposition

Suppose we use the T^2 statistic in (1) to construct a multivariate Shewhart chart for a bivariate normal process. Figure 1 contains the resultant elliptical control region for two positively correlated variables, x_1 and x_2. The separate univariate control limits for x_1 and x_2, which have been superimposed on the ellipse for comparison, form a "box." The chart signals when an observation plots outside the ellipse. This can occur when either or both of the individual variables are out of control and/or when the relationship between the two variables changes relative to the historical structure.

Individual variables which are out of control are easy to detect and interpret. A signaling point plots outside the box (and ellipse) in Figure 1 and signals on one or both univariate charts. Contrasting this situation are points that plot outside the ellipse but inside the box. These are the ones that make interpretation difficult as they indicate a counter-relationship problem (see, e.g., point A in Figure 1). Such points have observed values for each variable within the univariate control limits (box) but the bivariate T^2 charting statistic is outside the multivariate control limit (ellipse).

One method for interpreting such signals is to use the concept of the distance of an observation from the center of the data. For example, the center of the elliptical control region given in Figure 1 is located at the mean point, $(\bar{x}_1, \bar{x}_2)$. The squared Euclidean distance from the point A to this point is given by

$$d^2 = (x_1 - \bar{x}_1)^2 + (x_2 - \bar{x}_2)^2 . \tag{3}$$

It is easy to determine the effects of x_1 and x_2 on the distance measure in (3), as they are given by the two distance components on the right-hand side of (3). However, since these components ignore the effects of the variances and covariance of x_1 and x_2, the interpretations derived using them could be incorrect.

We know that a better statistical measure of distance is obtained using Mahalanobis' distance, which is the T^2 statistic in (1). The generalized distance from the point A in Figure 1 to the center of the ellipse is given by

$$\begin{aligned} T^2 &= \left(\mathbf{X} - \overline{\mathbf{X}}\right)' \mathbf{S}^{-1} \left(\mathbf{X} - \overline{\mathbf{X}}\right) \\ &= a_{11}(x_1 - \bar{x}_1)^2 + 2a_{12}(x_1 - \bar{x}_1)(x_2 - \bar{x}_2) \\ &\quad + a_{22}(x_2 - \bar{x}_2)^2 \end{aligned} \tag{4}$$

where a_{11}, a_{12}, and a_{22} are functions of the estimated variances and covariance of x_1 and x_2. Although the

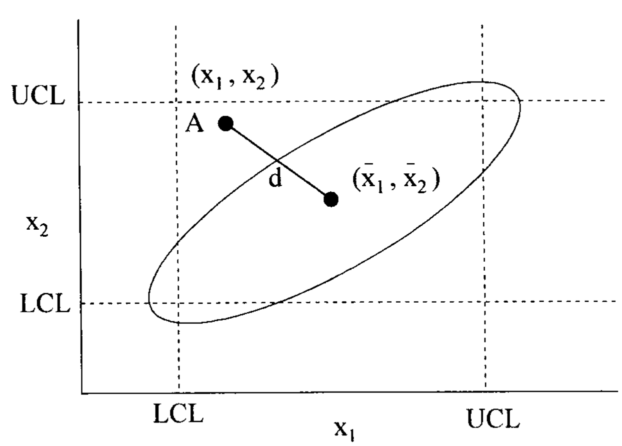

FIGURE 1. Bivariate Control Region with a Signaling Point.

T^2 statistic in (4) provides a useful statistical measure of distance and gives information on when an observation signals (i.e., due to the generalized distance from the center of the ellipse being large), the components on the right-hand side of (4) are not easily interpreted due to the cross product term involving both x_1 and x_2. Thus, a user cannot assess which variable is causing the signal.

Advocates of principal component analysis attempt to overcome the problems seen in (4) by transforming the x variables to their principal components. In such a setting, the generalized distance can be expressed as

$$T^2 = \frac{z_1^2}{\lambda_1} + \frac{z_2^2}{\lambda_2} \tag{5}$$

where

$$z_i = \mathbf{U}_i'(\mathbf{X} - \overline{\mathbf{X}}), \tag{6}$$

$i = 1, 2$, $\mathbf{U}_i$ is an orthonormal eigenvector of $\mathbf{S}$, and λ_i is the corresponding eigenvalue. This transformation produces principal components, z_i, that are uncorrelated and have a variance of λ_i. Since the generalized distance measure has been decomposed into independent components of the translated variables, z_1 and z_2, we can easily determine which of these new variables is causing a large T^2 value. This is accomplished by simply measuring the magnitude of each component on the right-hand side of (5).

The use of principal components, however, does not necessarily lead to interpretable components. To see this, let us re-express (6) in terms of the original x_1 and x_2 variables

$$z_1 = u_{11}(x_1 - \bar{x}_1) + u_{12}(x_2 - \bar{x}_2)$$

and

$$z_2 = u_{21}(x_1 - \bar{x}_1) + u_{22}(x_2 - \bar{x}_2)$$

where u_{ij} are elements of the corresponding eigenvectors of $\mathbf{S}$. It is evident that the principal components, z_1 and z_2, are linear combinations of x_1 and x_2. Unless these specific combinations are meaningful (see, e.g., Tracy, Young, and Mason (1995)), the interpretation of the components would be difficult. Thus, the problem remains of how to interpret a T^2 signal.

A different decomposition is needed that would have the feature of independent components, as in (5), but would be easily interpreted. The solution is given by the MYT decomposition. In this procedure, the T^2 statistic is decomposed into orthogonal components that are themselves generalized distance measures. For example, the T^2 value for the point A in Figure 1 can be expressed as

$$T^2 = \frac{(x_1 - \bar{x}_1)^2}{s_1^2} + \frac{(x_2 - \bar{x}_{2\cdot 1})^2}{s_{2\cdot 1}^2}, \tag{7}$$

or, alternatively, as

$$T^2 = \frac{(x_2 - \bar{x}_2)^2}{s_2^2} + \frac{(x_1 - \bar{x}_{1\cdot 2})^2}{s_{1\cdot 2}^2}, \tag{8}$$

where $s_{i\cdot j}^2$ is the estimated conditional variance of x_i given x_j, and $\bar{x}_{i\cdot j}$ is the estimated conditional mean of x_i given x_j. The two components in (7) give independent information on the effects of x_1 and of x_2 given x_1 on the signaling T^2. Similarly, the components in (8) provide information on the effects of x_2 and of x_1 given x_2 on the T^2 value. Taken together, these components can be used to determine whether an individual variable is out of control, and/or whether the relationship between the two variables has changed relative to that seen in the historical data.

Figure 2 illustrates this concept more clearly. For a given value of x_2, such as occurs at point A, the values of x_1 must be within the limits established by the elliptical control region. These are the values of x_1 given x_2 based on the information about variable relationships given in the historical data. As can be seen in Figure 2, the observed x_1 for point A is not in the required shaded region of the x_1 axis. Similarly, for a given value of x_1, such as occurs with point A, the values of x_2 are not in the required shaded region of the x_2 axis. The observation at A signals because something is incorrect in the relationship between x_1 and x_2.

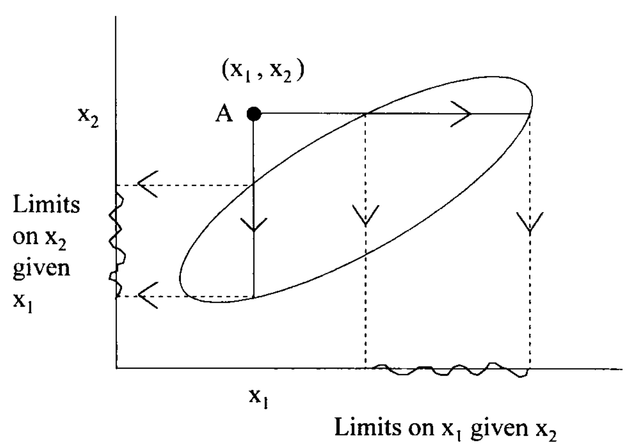

FIGURE 2. Conditional Bivariate Control Limits.

The MYT Decomposition

The T^2 statistic in (1) can be broken down or decomposed into p orthogonal components (Mason, Tracy, and Young (1995)). One form of the MYT decomposition is given by

$$T^2 = T_1^2 + T_{2\cdot 1}^2 + \cdots + T_{p\cdot 1,2,\ldots,p-1}^2. \quad (9)$$

The first term of this particular decomposition, T_1^2, is an unconditional Hotelling's T^2 for the first variable of the observation vector $\mathbf{X}$,

$$T_1^2 = \frac{(x_1 - \bar{x}_1)^2}{s_1^2}. \quad (10)$$

The general form of the other terms, referred to as conditional terms, is given as

$$T_{j\cdot 1,2,\ldots,j-1}^2 = \frac{(x_j - \bar{x}_{j\cdot 1,2,\ldots,j-1})^2}{s_{j\cdot 1,2,\ldots,j-1}^2}, \quad (11)$$

$j = 1, 2, \ldots, p$. This is the square of the j^{th} variable adjusted by the estimates of the mean and standard deviation of the conditional distribution of x_j given $x_1, x_2, \ldots, x_{j-1}$. (See Mason, Tracy, and Young (1995) for the notation concerning the calculation of these conditional estimates.)

The ordering of the p components in the vector $\mathbf{X}$ is not unique, and the one given above represents only one of the possible $p!$ different orderings of these components. Each ordering generates the same overall T^2 value, but provides a distinct partitioning of T^2 into p-orthogonal terms. Excluding redundancies, there are $p \times 2^{(p-1)}$ distinct components among the $p \times p!$ possible terms that should be evaluated for potential contribution to a signal.

To understand the difference between the decomposition specified in (9) and a different decomposition, consider the observation vector $\mathbf{X}$ where the p variables are in a specific order, such as $\mathbf{X} = (x_1, x_2, \ldots, x_p)'$. The sum of the components in (9), except the last term, is given as

$$T_1^2 + T_{2\cdot 1}^2 + \cdots + T_{p-1\cdot 1,2,\ldots,p-2}^2 = T^2 - T_{p\cdot 1,2,\ldots,p-1}^2,$$

and is the contribution of the subvector $(x_1, x_2, \ldots, x_{p-1})$ to the overall T^2. This is equivalent to the T^2 value that would be obtained if x_p had been excluded from the original study and only the first $p - 1$ variables were used in the computations. Note that this interpretation is dependent on the specific ordering of the variables. By changing the position of the last variable with one of the previous $p - 1$ variables, we would still obtain a T^2 based on $p - 1$ variables in the above sum but the interpretation would be different.

Interpretation of a Signal on a T^2 Component

Consider one of the p possible unconditional terms resulting from the decomposition of a T^2 statistic associated with an observation. The term,

$$T_j^2 = \frac{(x_j - \bar{x}_j)^2}{s_j^2}, \quad (12)$$

$j = 1, 2, \ldots, p$, is the square of a univariate t statistic for the observed value of the j^{th} variable of the vector $\mathbf{X}$ and produces a signal if that variable is out of control. Use of (12) to monitor the process is equivalent to the use of a univariate Shewhart control chart for the j^{th} variable. If univariate Shewhart charts were constructed for each of the p variables, the control limits from these charts plotted in a p-dimensional graph would produce a hyper-rectangular "box." If the observation vector is outside the "box", the signaling univariate T_j^2 values denote the out-of-control variables.

What happens when the overall T^2 signals but the observation is inside the hyper-rectangular box? As in the bivariate case, examination of the conditional terms of the decomposition of a T^2 statistic provides valuable information. In general, $T_{j\cdot 1,2,\ldots,j-1}^2$ is a standardized observation of the j^{th} variable adjusted by estimates of the mean and variance from the conditional distribution associated with $x_{j\cdot 1,2,\ldots,j-1}$. It can be used to check whether the raw (unstandardized) observation on the j^{th} variable is conforming to relationships with other variables as established by the historical situation, since the adjusted observation is most sensitive to changes in the covariance structure.

Information obtained from the conditional terms in the decomposition can be viewed from a regression analysis perspective. The estimated mean of x_j adjusted for $x_1, x_2, \ldots, x_{j-1}$ can be represented by the prediction equation

$$\bar{x}_{j\cdot 1,2,\ldots,j-1} = \bar{x}_j + \mathbf{B}_j' \left(\mathbf{X}^{(j-1)} - \overline{\mathbf{X}}^{(j-1)} \right), \quad (13)$$

where $\bar{x}_j$ is the sample mean of the n observations on the j^{th} variable, $\mathbf{B}_j$ is a $(j - 1)$-dimensional vector estimating the regression coefficients of the j^{th} variable regressed on the first $(j - 1)$ variables (for details, see Mason, Tracy, and Young (1995)), $\mathbf{X}^{(j-1)}$ is the observation vector with the j^{th} variable removed, and $\overline{\mathbf{X}}^{(j-1)}$ is the sample mean vector with the j^{th} element removed. These estimates are obtained using the historical data.

The right-hand side of (13) is a regression expression for x_j using the first $j-1$ variables as predictor variables. Using this information, we can re-express $T^2_{j\cdot 1,2,\ldots,j-1}$ in (11) as

$$T^2_{j\cdot 1,2,\ldots,j-1} = \frac{(x_j - \bar{x}_{j\cdot 1,2,\ldots,j-1})^2}{s_j^2(1 - R^2_{j\cdot 1,2,\ldots,j-1})} = \frac{\left(T_j - \widehat{T}_{j\cdot 1,2,\ldots,j-1}\right)^2}{1 - R^2_{j\cdot 1,2,\ldots,j-1}} \tag{14}$$

where $\widehat{T}_{j\cdot 1,2,\ldots,j-1} = \mathbf{B}_j'\left(\mathbf{X}^{(j-1)} - \overline{\mathbf{X}}^{(j-1)}\right)/s_j$ is viewed as a predicted value of the unconditional term, T_j, and $R^2_{j\cdot 1,2,\ldots,j-1}$ is the squared multiple correlation coefficient between x_j and x_1, x_2, ..., x_{j-1} (see, e.g., Rencher (1993)). If x_j is not correlated with x_1, x_2, ..., x_{j-1}, the expression in (14) reduces to the univariate T_j^2 in (12). Otherwise, the conditional terms in a T^2 decomposition explain how well a future observation on a particular variable is in agreement with the value predicted by a set of the other variate values of the vector, using the covariance structure established in the historical data set.

Unless the denominator in (14) is very small, as occurs when R_j^2 is near 1, the "largeness" of the conditional T^2 term will be due to the numerator, which is a function of the agreement between the observed and predicted T values. For example, consider an observation X that is inside the "box" and suppose there is significant disagreement in magnitude between an observed unconditional T_j value and the corresponding $\widehat{T}_{j\cdot 1,2,\ldots,j-1}$ value. This implies that the standardized observation on this particular component is below or above what was expected as established by the historical situation using the first $j-1$ predictor values from the $\mathbf{X}$ vector.

To better understand the result in (14), consider a bivariate situation. In this case, there are two conditional T^2 terms whose square roots are given by

$$T_{2\cdot 1} = \frac{x_2 - \bar{x}_{2\cdot 1}}{s_{2\cdot 1}} = \frac{r_{2\cdot 1}}{s_2\sqrt{1 - R^2_{2\cdot 1}}} \tag{15}$$

$$T_{1\cdot 2} = \frac{x_1 - \bar{x}_{1\cdot 2}}{s_{1\cdot 2}} = \frac{r_{1\cdot 2}}{s_1\sqrt{1 - R^2_{1\cdot 2}}} \tag{16}$$

where $r_{2\cdot 1} = x_2 - \bar{x}_{2\cdot 1}$ and $r_{1\cdot 2} = x_1 - \bar{x}_{1\cdot 2}$ are residuals from the respective regression fits of x_2 on x_1 and x_1 on x_2. These residuals are illustrated in Figures 3 and 4.

Notice that the two conditional values in (15) and (16), apart from the $R^2_{i\cdot j}$ term, are actually standardized residuals having the form of $r_{i\cdot j}/s_i$. It is in this sense that we obtain the standardized residual form for the conditional T^2 given in (14). When the residuals (after standardizing) in Figures 3 and 4 are large, the conditional T^2 terms signal. This would occur only when the observed value of x_1 (or x_2) differs from the value predicted by x_2 (or x_1) using the historical data.

It is easy to generalize this geometric argument. When the conditional T^2 term in (14) involves many variables (i.e., $p > 2$), its size is directly related to the magnitude of the standardized residual resulting from the prediction of x_j using x_1, x_2, ..., x_{j-1} and the historical data set. When the (standardized) residual is large, the conditional T^2 signals.

The above results indicate that a T^2 signal can be produced by an observation that has an individual variable that is out of control. A signal of this form is based solely on the observed value of the variable and can be detected with the unconditional univariate T_j^2 terms. The relationship of the specified variable with the other variables, however, is not taken into consideration. A second way a T^2 signal may occur is for something to go astray with the relationships between subsets of the various variables. This situation can be determined by examination of the conditional T^2 terms. A signaling value indicates that a contradiction with the historical relationship between the variables has occurred either (1) due to a standardized component value that is significantly larger or smaller than that predicted by a subset of

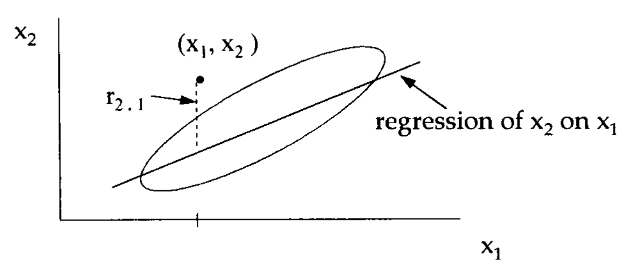

FIGURE 3. Residual from Regression of x_2 on x_1.

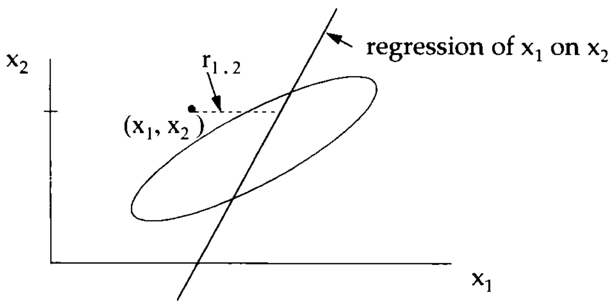

FIGURE 4. Residual from Regression of x_1 on x_2.

the remaining variables, or (2) due to a standardized component value that is marginally smaller or larger than that predicted by a subset of the remaining variables when there is a very severe collinearity among the variables. Thus, a signal results when an observation on a particular variable, or set of variables, is out of control, and/or when observations on a set of variables are counter to the relationship established by the historical data.

Data Examples

Consider the interpretation of a signal when we have only two process variables. We use this simple case to illustrate our interpretation procedure as it is easiest to visualize graphically. Suppose $\mathbf{X} = (x_1, x_2)'$ so that there are only four terms available for the overall decomposition: T_1^2, T_2^2, $T_{1\cdot 2}^2$ and $T_{2\cdot 1}^2$. The T^2 statistic can be written as either

$$T^2 = T_1^2 + T_{2\cdot 1}^2,$$

or,

$$T^2 = T_2^2 + T_{1\cdot 2}^2,$$

and it represents the generalized distance from the point (x_1, x_2) to its mean $(\bar{x}_1, \bar{x}_2)$. These two decompositions express this distance as a sum of the generalized distance one variable is from its mean, denoted by the unconditional T_j^2 term, plus the generalized distance the other variable is from its conditional mean, denoted by the conditional term, $T_{i\cdot j}^2$. Examining these component parts of the decomposition can give additional insight into the causes of an observation producing a signal.

An example of a bivariate process, taken from the chemical industry, occurs when an electric current is passed through an electrolyzer containing brine in order to decompose it into such by-products as caustic and hydrogen, oxygen, and chlorine gas. Suppose the two process variables to be monitored include NaOH (caustic), labeled x_1, and NaCL (salt), labeled x_2. We collected 416 "clean" bivariate observations from such a process in order to form an historical data set to be used in constructing a bivariate control region. This data set, which has been coded for proprietary reasons, is described below. The two process variables, x_1 and x_2, are moderately correlated in the historical data set, and have a correlation of 0.57. The sample mean vector, $\overline{\mathbf{X}}$, is given by

$$\overline{\mathbf{X}} = \begin{pmatrix} 143.94 \\ 200.83 \end{pmatrix},$$

and the sample covariance matrix is

$$\mathbf{S} = \begin{pmatrix} 225.80 & 91.81 \\ 91.81 & 116.37 \end{pmatrix}.$$

Using the distribution given in (2) and a significance level of 0.05, the control region is defined by the following equation:

$$\begin{pmatrix} x_1 - 143.94 \\ x_2 - 200.83 \end{pmatrix}' \begin{pmatrix} 225.80 & 91.81 \\ 91.81 & 116.37 \end{pmatrix}^{-1} \times \begin{pmatrix} x_1 - 143.94 \\ x_2 - 200.83 \end{pmatrix} = 6.06. \quad (17)$$

Figure 5 illustrates the bivariate elliptical control region obtained using (17). Plotted in the figure are the two regression equations of x_1 on x_2, and of x_2 on x_1, which were constructed using the historical data set and the formula given in (13). The resulting two slopes, $\mathbf{B}_1$ and $\mathbf{B}_2$, associated with these prediction equations are listed in Table 1. Surrounding the control region are four signaling points, labeled A, B, C, and D, which illustrate the possible interpretations associated with a T^2 statistic.

The values of the unconditional and conditional T^2 terms associated with these four points are given in Table 2. Point A indicates an observation which is located inside the univariate control limit for x_1 but outside the univariate control limit for x_2 as well

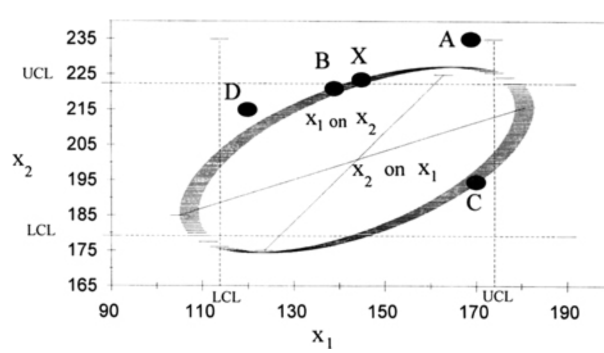

FIGURE 5. Bivariate Control Region, $r = 0.57$.

TABLE 1. Predictor Terms for Data Example, $r = 0.57$

Response	Predictor	Slope	$R^2_{i \cdot j}$
x_1	x_2	0.79	0.32
x_2	x_1	0.41	0.32

as outside the bivariate elliptical control region. Because the point is outside the box formed using the univariate control limits for x_1 and x_2, we would not need to decompose the corresponding T^2 value. Instead, our initial step would be to examine the x_2 value of A and try to bring it into control.

Points B, C, and D illustrate observations that are signaling because they are inside the univariate control limits for both x_1 and x_2 but outside the elliptical control region. For these types of points, the T^2 decomposition can be very helpful. Although all three points have a significant overall T^2 value, none of them has a significant T_1^2 or T_2^2 value. However, point B has a significant $T^2_{2 \cdot 1}$ value, point C has a significant $T^2_{1 \cdot 2}$ value, and point D has both significant $T^2_{1 \cdot 2}$ and $T^2_{2 \cdot 1}$ values. Our interpretation of these three signals is that they occur because one or more of the components of the corresponding observations is counter to the relationship indicated by the historical data.

An examination of the values in Table 3, which contains the predicted and observed T_j values associated with the conditional T^2 terms, for points B, C, and D, indicates the cause of the signaling conditional T^2 values. For Point B, the signal results because the observed T_2 value of 1.87 is larger than the predicted value of -0.19 obtained using the historical data. For point C, the observed T_1 value of 1.73 is larger than the predicted value of -0.33. For point D, T_1 is smaller and T_2 is larger than the corresponding predicted values. Thus, we have been able to determine that the cause of the signals is an observation that has one or more components above or below the values predicted by the historical data. To correct the problem, we would need to examine the x_2 value of point B, the x_1 value of point C, and the x_1 and x_2 values of point D.

TABLE 2. Decomposition Terms for Data Example, $r = 0.57$

Point	T^2	T_1^2	T_2^2	$T^2_{1 \cdot 2}$	$T^2_{2 \cdot 1}$
A	10.05*	2.78	10.03*	0.02	7.27*
B	6.33*	0.11	3.49	2.83	6.22*
C	6.63*	3.01	0.34	6.29*	3.62
D	9.76*	2.54	1.73	8.03*	7.22*

*Denotes significance at 0.05 level.

TABLE 3. Predicted and Observed Values Associated with Conditional T^2 Terms

Point	T_1	$\widehat{T}_{1 \cdot 2}$	$T_1 - \widehat{T}_{1 \cdot 2}$	T_2	$\widehat{T}_{2 \cdot 1}$	$T_2 - \widehat{T}_{2 \cdot 1}$
B	0.33	1.06	-0.73	1.87	-0.19	2.06*
C	1.73	-0.33	2.06*	-0.59	0.98	-1.57
D	-1.59	0.74	-2.33*	1.31	-0.90	2.21*

*Denotes residual > 2.

In monitoring the brine-conversion process described by the control region in (17), a new observation, given by

$$\mathbf{X} = \begin{pmatrix} 145.0 \\ 223.5 \end{pmatrix} \tag{18}$$

was taken independent of the historical data set. The observation given in equation (18) yielded an overall T^2 value of 6.26, which signaled need of interpretation. Table 4 contains the conditional and unconditional values associated with this observation. The unconditional T_2^2 term is significant, but not the unconditional T_1^2, indicating that the observation on x_2, which represents NaCL, is outside its univariate control limits. The interpretation is similar to that given for point A; the point $\mathbf{X}$ is outside the box formed by the univariate control limits on x_1 and x_2, and thus we do not need to continue decomposing the associated T^2 value.

The above example involved the monitoring of a process where the two variables were moderately correlated. In order to observe the effect a strong bi-

TABLE 4. Decomposition of Signaling Point

Point	T^2	T_1^2	T_2^2	$T^2_{1 \cdot 2}$	$T^2_{2 \cdot 1}$
$\mathbf{X}$	6.26*	0.005	4.42*	1.84	6.26*

T_1	$\widehat{T}_{1 \cdot 2}$	$T_1 - \widehat{T}_{1 \cdot 2}$	T_2	$\widehat{T}_{2 \cdot 1}$	$T_2 - \widehat{T}_{2 \cdot 1}$
0.071	1.84	-1.77	2.10	0.040	2.06**

*Denotes significance at 0.05 level.

**Denotes residual > 2.

variate correlation might have on the terms in a T^2 decomposition, suppose we now monitor the chlorine gas, labeled x_1, and the oxygen gas, labeled x_2, produced in the previous electrolyzer process example. We thus have 416 bivariate observations and we will use them to form an historical data set to be used in constructing an elliptical control region. This data set, which has been coded for proprietary reasons, is described below. The correlation between the two process variables is 0.99. The sample mean vector, $\overline{\mathbf{X}}$, is given by

$$\overline{\mathbf{X}} = \begin{pmatrix} 26.1 \\ 94.8 \end{pmatrix},$$

and the sample covariance matrix is given by

$$\mathbf{S} = \begin{pmatrix} 156.25 & 91.58 \\ 91.58 & 54.76 \end{pmatrix}.$$

Using the distribution given in (2) and a significance level of 0.05, the control region is defined by the following equation:

$$\begin{pmatrix} x_1 - 26.1 \\ x_2 - 94.8 \end{pmatrix}' \begin{pmatrix} 156.25 & 91.58 \\ 91.58 & 54.76 \end{pmatrix}^{-1} \begin{pmatrix} x_1 - 26.1 \\ x_2 - 94.8 \end{pmatrix} = 6.06. \quad (19)$$

Figure 6 illustrates the bivariate elliptical control region obtained using (19). Plotted in the figure are the two regression equations of x_1 on x_2, and of x_2 on x_1, which were constructed using the above historical data set and the formula given in (13). The resulting two slopes, $\mathbf{B}_1$ and $\mathbf{B}_2$, associated with these equations are listed in Table 5. Surrounding the control region are four signaling points, labeled A, B, C, and D, which illustrate the various interpretations associated with a T^2 statistic.

Table 6 contains the conditional and unconditional T^2 terms associated with these four points.

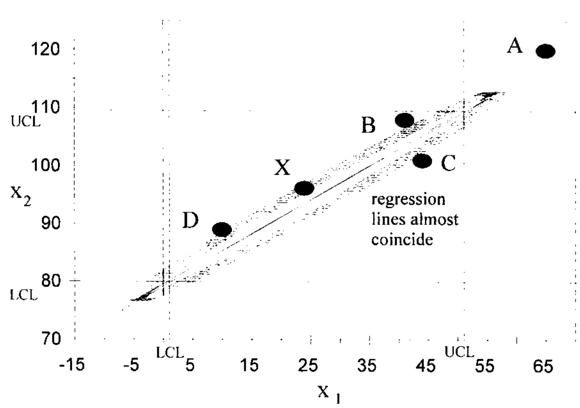

FIGURE 6. Bivariate Control Region, $r = 0.99$.

TABLE 5. Predictor Terms for Data Example, $r = 0.99$

Response	Predictor	Slope	$R^2_{i \cdot j}$
x_1	x_2	1.67	0.98
x_2	x_1	0.59	0.98

Point A is outside both univariate control limits, and this is reflected by the large unconditional T^2 terms. As occurred in the first example, we would not need to decompose the corresponding T^2 value as the problem lies in the large separate values of x_1 and x_2.

Points B, C, and D are all inside the box formed by the univariate control limits on x_1 and x_2 but outside the elliptical control region. Consequently, their unconditional T^2 terms are small but their conditional T^2 terms are large. The cause of these large values, however, is different than that noted for the corresponding points in the first example. For this chlorine-oxygen gas data, the elliptical control region, as illustrated in Figure 6, is very narrow, and the two regression lines of x_1 on x_2, and of x_2 on x_1, are so close that they almost coincide. Because of this, all three points appear to be near both lines. This result is confirmed in Table 7 for points B, C and D as each has very small deviations between either T_1 or T_2 and their corresponding predicted values.

The cause of the large conditional T^2 values for points B and C can be traced to the large $R^2_{i \cdot j}$ values in Table 5. These correlations are an integral part of the formulas in (15) and (16), and dominate the value of the difference between the observed and predicted T^2 values. This result suggests that there is a need to eliminate the severe collinearity between x_1 and x_2 in the historical data set before constructing the control region. Similar observations on screening the

TABLE 6. Decomposition Terms for Data Example, $r = 0.99$

Point	T^2	T^2_1	T^2_2	$T^2_{1\cdot 2}$	$T^2_{2\cdot 1}$
A	14.99*	9.68	11.60*	3.40	5.32*
B	19.83*	1.42	3.18	16.65*	18.41*
C	19.04*	2.05	0.70	18.34*	16.99
D	13.86*	1.66	0.62	13.24*	12.20*

*Denotes significance at 0.05 level.

TABLE 7. Predicted and Observed Values Associated with Conditional T^2 Terms

Point	T_1	$\widehat{T}_{1\cdot 2}$	$T_1 - \widehat{T}_{1\cdot 2}$	T_2	$\widehat{T}_{2\cdot 1}$	$T_2 - \widehat{T}_{2\cdot 1}$
B	1.19	1.77	−0.58	1.78	1.18	0.60
C	1.43	0.83	0.60	0.84	1.42	−0.58
D	−1.29	−0.78	−0.51	−0.78	−1.28	0.50

historical data for collinearities have been noted by Kourti and MacGregor (1996).

In monitoring the chlorine-oxygen gas example described by the control region in (19), a new observation, given by

$$\mathbf{X} = \begin{pmatrix} 24.0 \\ 96.2 \end{pmatrix} \tag{20}$$

was taken independent of the historical data set. The observation given in equation (20) yielded an overall T^2 value of 6.41, which signaled that the process was out of control.

Table 8 contains the conditional and unconditional T^2 values associated with this observation. As with point D in Table 7, both unconditional T^2 values were not significant while both of the conditional T^2 values were significant. The interpretation is similar to that given for point D; the point is out of control because the chlorine and oxygen gas values are simultaneously too large. However, a more severe problem is the severe collinearity between the chlorine and oxygen gas values in the historical data set. If possible, this collinearity should be eliminated and the elliptical control region in Figure 6 should be reconstructed before trying to modify the process to correct for this out-of-control point.

Computational Scheme

A primary consideration in the decision to use a particular control procedure is ease of computation. With multivariate control procedures, interpretation

TABLE 8. Decomposition of Signaling Point

Point	T^2	T_1^2	T_2^2	$T_{1\cdot 2}^2$	$T_{2\cdot 1}^2$
$\mathbf{X}$	6.41*	0.028	0.036	6.38*	6.39*

T_1	$\widehat{T}_{1\cdot 2}$	$T_1 - \widehat{T}_{1\cdot 2}$	T_2	$\widehat{T}_{2\cdot 1}$	$T_2 - \widehat{T}_{2\cdot 1}$
−0.168	0.187	−0.355	0.189	−0.166	0.355

*Denotes significance at 0.05 level.

TABLE 9. Unique MYT Decomposition Terms

p	# of unique terms
2	4
3	12
4	32
5	80
10	5120
15	245760
20	10485760

efforts in particular may require numerous computations, a fact which might initially discourage practitioners. The MYT decomposition of the T^2 statistic has been shown to be a great aid in the interpretation of signaling T^2 values, but the number of unique terms can be large, particularly when p exceeds 10. The magnitude of the problem, illustrated in Table 9, has been noted by other authors (see, e.g., Kourti and MacGregor (1996)). It has also led to the development of computer programs that can rapidly produce the significant components of the decomposition (see, e.g., Langley, Young, Tracy, and Mason (1995)). The following is a sequential computational scheme that has the potential of further reducing the computations to a reasonable number when the overall T^2 signals.

Step 1. Compute the individual T^2 statistic for every component of the $\mathbf{X}$ vector. Remove variables whose observations produce a significant T_i^2. The observations on these variables are out of individual control and it is not necessary to check how they relate to the other observed variables. With significant variables removed we have a reduced set of variables. Check the subvector of the remaining k variables for a signal. If no signal remains, we have located the source of the problem.

Step 2. (Optional but useful for very large p.) Examine the correlation structure of the reduced set of variables. Remove any variable having a very weak correlation (0.3 or less) with all the other variables. The contribution of a variable that falls in this category is measured by the T_i^2 component.

Step 3. If a signal remains in the subvector of k variables not deleted, compute all $T_{i\cdot j}^2$ terms. Remove from study all pairs of variables, (x_i, x_j), that have a significant $T_{i\cdot j}^2$ term. This indicates that something is wrong with the bivariate relationship. When this occurs it will further reduce the set of variables under consideration. Examine all removed variables for the cause of the signal. Compute the T^2 value for the remaining subvector. If no signal is present, the source of the problem is with the bivariate relationships and those variables that were out of individual control.

Step 4. If the subvector of the remaining variables still contains a signal, compute all $T^2_{i \cdot j,k}$ terms. Remove any triple, (x_i, x_j, x_k), of variables that show significant results and check the remaining subvector for a signal.

Step 5. Continue computing the higher-order terms in this fashion until there are no variables left in the reduced set. The worst case situation is that all unique terms will have to be computed.

Let us apply this computational scheme to the simulated data from Hawkins (1991) that is described in Mason, Tracy, and Young (1995). Measurements were taken on five dimensions of switch drums: the inside diameter of the drum, x_1, and the distances from the head to the edges of four sectors of the drum, x_2, x_3, x_4, and x_5. A signaling observation from this situation yielded a $T^2 = 22.88$. With $p = 5$, there are $5 \times 24^4 = 80$ distinct components that could be evaluated in decomposing the T^2 to determine the cause of the signal. Table 10 contains the 31 significant terms out of 80 and indicates the cause of the problem exists with the relationship between x_1 and the other variables, and between x_5 and its relationship to x_1 as well as to x_4.

TABLE 10. Significant Decomposition Components for Hawkins' Signaling Observation

Component	Value	Component	Value
T^2_1	7.61	T^2_3	8.10
$T^2_{1\cdot 2}$	8.90	$T^2_{3\cdot 14}$	6.00
$T^2_{1\cdot 3}$	14.96	$T^2_{3\cdot 12}$	7.06
$T^2_{1\cdot 4}$	9.41	$T^2_{3\cdot 124}$	6.70
$T^2_{1\cdot 5}$	15.62	$T^2_{5\cdot 1}$	11.87
$T^2_{1\cdot 23}$	15.78	$T^2_{5\cdot 4}$	4.43
$T^2_{1\cdot 24}$	9.33	$T^2_{5\cdot 12}$	10.48
$T^2_{1\cdot 25}$	15.98	$T^2_{5\cdot 14}$	11.51
$T^2_{1\cdot 34}$	15.18	$T^2_{5\cdot 24}$	4.73
$T^2_{1\cdot 35}$	15.10	$T^2_{5\cdot 34}$	4.66
$T^2_{1\cdot 45}$	16.49	$T^2_{5\cdot 123}$	4.93
$T^2_{1\cdot 234}$	15.86	$T^2_{5\cdot 124}$	11.85
$T^2_{1\cdot 235}$	16.79	$T^2_{5\cdot 134}$	6.89
$T^2_{1\cdot 245}$	16.45	$T^2_{5\cdot 234}$	5.66
$T^2_{1\cdot 345}$	17.41	$T^2_{5\cdot 1234}$	6.17
$T^2_{1\cdot 2345}$	16.37		

TABLE 11. Partial T^2 Decomposition for Hawkins' (1991) Data

Variable (x_i)	T^2_i
x_1	7.61*
x_2	0.67
x_3	0.76
x_4	0.58
x_5	3.87

*Denotes significance at 0.05 level, based on one-sided upper critical value = 4.28.

Suppose the Hawkins' (1991) data is re-examined using our computational scheme. At Step 1, the five individual T^2 statistics would be computed. These are given in Table 11. Only T^2_1 is significant, so variable 1 is removed from the analysis. After removing x_1 from the data vector, the subvector is still significant ($T^2 - T^2_1 = 22.88 - 7.61 = 16.37$). Thus, the twelve $T^2_{i \cdot j}$ terms that do not involve x_1 must be computed. Of these, only $T^2_{5\cdot 4}$ is significant, so x_4 and x_5 are removed from the analysis. At this time, the subvector involving x_2 and x_3 is not significant so the calculations stop. The interpretation is that x_1 is out of individual control and that the observed value for x_5 is not what would be predicted by the observed value of x_4 according to the historical data. The computational scheme was very efficient and reduced the number of required calculations from 80 terms to only 17 terms.

Summary and Discussion

Additional details about interpreting the terms involved in the decomposition of a Hotelling's T^2 statistic have been presented in this paper. The T^2 components were shown to be generalized distances to the center of the data, and thus reflective of their separation from the sample center. The conditional terms were shown to be especially informative as they mirror the residual in the regression fit of one variable to a subset of the remaining variables, and, in addition, they can be used as charting statistics to monitor conditional trends.

The interpretation of the unconditional T_j^2 terms of the decomposition is straightforward as they measure whether an individual observation is within control. A signaling conditional term indicates that the observation on the corresponding set of variables is counter to the relationship established by the historical data. This occurs because the standardized component value is larger or smaller than that predicted by the subset, or because of a severe collinearity between a subset of the variables. This latter situation can be easily eliminated by properly screening the historical data set and eliminating redundant variables. The former case, however, requires process intervention to correct the out-of-control situation.

A sequential computation scheme was introduced that has the potential of reducing the number of required T^2 terms that need to be computed in a decomposition. The procedure moves from lower-order terms, (i.e., unconditional) to bivariate conditional terms to higher-order conditional terms. Along this forward path, significant variables are eliminated from other decompositions. The high processing speed of personal computers and this sequential computation scheme combine to make a useful and practical tool for practitioners.

Whether the T^2 statistic is chosen as the primary charting statistic or if some other multivariate charting procedure is used (such as the multivariate cumulative sum (MCUSUM) or multivariate exponentially weighted moving average (MEWMA)) the T^2 decomposition procedure described earlier in this paper can be very beneficial in interpreting control chart signals. In addition, while other decompositions could be posed for the T^2 statistic, the procedure given here lends itself most readily to easy interpretation. It is especially sensitive to changes in the linear relationships between and among variable subsets. This, in turn, aids the practitioner in quickly isolating the variable or variable relationships causing the signal. However, while this technique will identify the variable, or set of variables causing the signal, it does not necessarily distinguish between mean shifts and shifts in the variability of these variables. This is an area for further research.

References

HAWKINS, D. M. (1991). "Multivariate Quality Control Based on Regression-Adjusted Variables". *Technometrics* 33, pp. 61-75.

JACKSON, J. E. (1985). "Multivariate Quality Control". *Communications in Statistics - Theory and Methods* 14, pp. 2657-2688.

JACKSON, J. E. (1991). *A User's Guide to Principal Components*. John Wiley & Sons, Inc., New York, NY.

KOURTI, T. and MACGREGOR, J. F. (1996). "Multivariate SPC Methods for Monitoring Process and Product Performance". *Journal of Quality Technology* 28, pp. 409-428.

LANGLEY, M. P.; YOUNG, J. C.; TRACY, N. D.; and MASON, R. L. (1995). "A Computer Program for Monitoring Multivariate Process Performance". Proceedings of the Section on Quality and Productivity, American Statistical Association, Alexandria, VA, pp. 122-123.

MASON, R. L.; TRACY, N. D.; and YOUNG, J. C. (1995) "Decomposition of T^2 for Multivariate Control Chart Interpretation". *Journal of Quality Technology* 27, pp. 99-108.

RENCHER, A. C. (1993). "The Contribution of Individual Variables to Hotelling's T^2, Wilks' Λ, and R^2". *Biometrics* 49, pp. 479-489.

TRACY, N. D.; YOUNG, J. C.; and MASON, R. L. (1995). "A Bivariate Control Chart for Paired Measurements". *Journal of Quality Technology* 27, pp. 370-376.

Key Words: *Hotelling's T^2 Statistic, Multiple Regression, Multivariate Control Charts.*